

WHAT IS CLAIMED IS:

1. A computerized method for identifying peaks corresponding to glycans from a mass spectrum, comprising:
receiving not less than one glycan spectrum from a mass spectrometer, wherein said not less than one glycan spectrum includes peaks having a measured mass;
assigning glycan identifications to said peaks; and
reporting said peak assignments.
2. The method for identifying peaks corresponding to glycans according to claim 1, further comprising constructing a monosaccharide set table having a plurality of isomers corresponding to glycans.
3. The method for identifying peaks corresponding to glycans according to claim 2, wherein constructing said monosaccharide set table comprises:
constructing a glycan/monosaccharide set chart, wherein each row represents a set of monosaccharides;
applying combination ranges for said monosaccharides;
developing a rule set, wherein said rules specify monosaccharide combination limitations;
eliminating each of said monosaccharide rows not satisfying said rule set; and
computing glycan isomer mass and glycan isotope frequency.
4. The method for identifying peaks corresponding to glycans according to claim 1, wherein assigning glycan identifications comprises:
calibrating said received glycan spectrum; and
matching isotopes from said monosaccharide set table to said peaks within said glycan spectrum.

5. The method for identifying peaks corresponding to glycans according to claim 4, wherein calibrating said received glycan spectrum comprises setting said calibration explicitly.

6. The method for identifying peaks corresponding to glycans according to claim 4, wherein matching isotopes comprises:

selecting the isotope with the highest expected frequency for each said monosaccharide;

searching said spectrum for a peak within an acceptable tolerance of said isotope; and

selecting said peak having the best isotope envelope.

7. The method for identifying peaks corresponding to glycans according to claim 4, further comprising performing a quality assessment, wherein said quality assessment determines the likelihood that said peak assignment is correct.

8. The method for identifying peaks corresponding to glycans according to claim 7, wherein performing said quality assessment comprises:

measuring proximity of said measured mass of a selected peak to the theoretical mass of the glycan;

computing said isotope envelopes; and

examining the peak height at a peak height mass minus one position.

9. The method for identifying peaks corresponding to glycans according to claim 4, further comprising performing spectrum combination, wherein said spectrum combination includes combining the information from a plurality of spectra.

10. The method for identifying peaks corresponding to glycans according to claim 1, wherein said reporting of said peak assignments comprises not less than one family

report, wherein said family comprises a sequence of spectrum peaks, wherein the label for each succeeding peak contains not less than one more monosaccharide than the label of the preceding peak.

11. The method for identifying peaks corresponding to glycans according to claim 1, wherein said glycan identifications comprise a plurality of cartoons, wherein said cartoons comprise symbolic representations of said rows from said monosaccharide table.

12. A computerized system for identifying peaks corresponding to glycans from a mass spectrum, comprising:

- a spectrum receiver for transmitting not less than one spectrum file to the system, wherein said spectrum file includes not less than one set of masses or mass ranges and the ion frequency for each said mass or mass range;

- a maketable module for constructing a monosaccharide set table, wherein each row of said monosaccharide set table represents a set of monosaccharides;

- an identification module for developing a listing of mass peaks in said spectrum which match an isomer from said monosaccharide set table;

- a summary module for structuring a glycan report; and

- a plurality of memory modules, comprising:

- a monosaccharide set table module;

- a peak identification file module;

- a cartoon dictionary, wherein said cartoon dictionary includes symbolic representations of rows of said monosaccharide set table; and

- a glycan report file module.

13. A computerized system for identifying peaks corresponding to glycans according to claim 12, further comprising a family module for structuring not less than one family report, wherein said family comprises a sequence of spectrum peaks, wherein the label

for each succeeding peak contains not less than one more monosaccharide than the label of the preceding peak.

14. A computerized system for identifying peaks corresponding to glycans according to claim 12, wherein said monosaccharide set table construction comprises:

means for constructing a glycan/monosaccharide set chart, wherein each row represents a set of monosaccharides;

means for applying combination ranges for said monosaccharides;

means for developing a rule set, wherein said rules specify monosaccharide combination limitations;

means for eliminating each of said monosaccharide rows not satisfying said rule set; and

means for computing glycan isomer mass and glycan isotope frequency.

15. A computerized system for identifying peaks corresponding to glycans according to claim 12, wherein said identification module comprises:

means for calibrating said received glycan spectrum; and

means for matching isotopes from said monosaccharide set table to said peaks within said glycan spectrum.

16. A computerized system for identifying peaks corresponding to glycans according to claim 15, wherein matching isotopes comprises:

means for selecting the isotope with the highest expected frequency for each said monosaccharide;

means for searching said spectrum for a peak within an acceptable tolerance of said isotope; and

means for selecting said peak having the best isotope envelope.

17. A computerized system for identifying peaks corresponding to glycans according to claim 15, further comprising means for performing a quality assessment, wherein said quality assessment determines the likelihood that said perk assignment is correct.

18. A computerized system for identifying peaks corresponding to glycans according to claim 17, wherein means for performing said quality assessment comprises:

means for measuring proximity of said measured mass of a selected peak to the theoretical mass of the glycan;

means for computing said isotope envelopes; and

means for examining the peak height at a peak height mass minus one position.

19. A computerized system for identifying peaks corresponding to glycans according to claim 15, further comprising means for performing spectrum combination, wherein said spectrum combination includes combining the information from a plurality of spectra.

20. A computerized system for identifying peaks corresponding to glycans according to claim 16, further comprising means for assigning glycan identifications, wherein said glycan identifications comprise cartoons.

21. An article of manufacture comprising a computer usable medium having computer readable program code embodied in said medium which, when said program code is executed by said computer causes said computer to perform method steps for identifying peaks corresponding to glycans from a mass spectrum, comprising:

receiving not less than one glycan spectrum from a mass spectrometer, wherein said not less than one glycan spectrum includes peaks having a measured mass;

assigning glycan identifications to said peaks; and

reporting said peak assignments.